Computational and Experimental Method for Evaluating the Reactivity of Substituted Toluene Diamines and Azo Compounds in the Reactions of Amine and Anhydride Curing of Epoxy Resins

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Abstract—The optimization of the molecular structure of substituted 3,5-toluylene diamines was carried out by the ab initio method, which made it possible to calculate the volume of stretching vibrations and the steric factor of the ethyl and methylthiol substituents on the basis of the data obtained on the bond lengths and bond angles. A linear dependence of the total steric factor of substituents in the molecules of substituted 3,5-toluylene diamines on the activation energy of the reaction of their polyaddition with novolac epoxy resin was established. For 4-phenylazophenol, 4-methoxyazobenzene, 4-phenylazo-*N,N′*-dimethylaniline, 1-(2-pyridylazo)-2-naphthol, phenylazo-4-naphthylamine, studied as catalysts for the polyaddition of isomethyltetrahydrophthalic anhydride to epoxy resin, dependence of the activation energy on the value of the electron density is observed at the nitrogen atom of the azo group. The derived linear dependences evidence the established latency of epoxy binders, which depends mainly on hardeners and catalysts. Using a computational and experimental method for evaluating the reactivity of hardeners and catalysts, heat-resistant polymers and composites with good physical-mechanical and thermomechanical characteristics were produced, which meet modern requirements for products operating in a wide temperature range.

Keywords: epoxy binder, curing catalyst, electronic structure, steric factor, polymer composite

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